

10/820,216

=> d his

(FILE 'HOME' ENTERED AT 15:52:55 ON 15 FEB 2006)

FILE 'REGISTRY' ENTERED AT 15:53:05 ON 15 FEB 2006

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 39 S L1 SSS FUL

FILE 'CAPLUS' ENTERED AT 15:53:53 ON 15 FEB 2006

L4 25 S L3

L5 ANALYZE L4 1- RN HIT : 39 TERMS

FILE 'REGISTRY' ENTERED AT 15:54:07 ON 15 FEB 2006

L6 1 S 144912-63-0/RN

L7 38 S L3 NOT L6

FILE 'CAPLUS' ENTERED AT 15:56:04 ON 15 FEB 2006

L8 17 S L7

L9 18 S L6

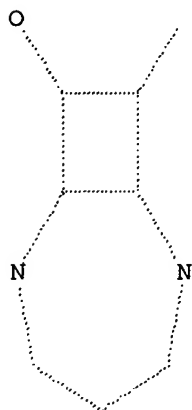
L10 10 S L8 AND L9

L11 17 S L8 OR L10

=> d l1

L1 HAS NO ANSWERS

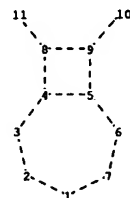
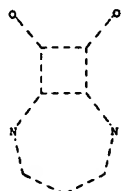
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d l6

YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y



chain nodes :

10 11

ring nodes :

1 2 3 4 5 6 7 8 9

chain bonds :

8-11 9-10

ring bonds :

1-2 1-7 2-3 3-4 4-5 4-8 5-6 5-9 6-7 8-9

exact/norm bonds :

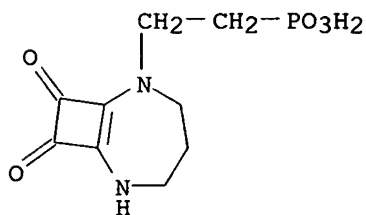
1-2 1-7 2-3 3-4 4-5 4-8 5-6 5-9 6-7 8-9 8-11 9-10

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS

10/820,216

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
RN **144912-63-0** REGISTRY
ED Entered STN: 15 Dec 1992
CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2,6-Diazabicyclo[5.2.0]nonane, phosphonic acid deriv.
OTHER NAMES:
CN EAA 090
CN Perzinfotel
CN Way 126090
FS 3D CONCORD
MF C9 H13 N2 O5 P
CI COM
SR CA
LC STN Files: ADISINSIGHT, BIOSIS, CA, CAPLUS, CASREACT, IMSDRUGNEWS, IMSRESEARCH, IPA, PHAR, PROMT, PROUSDDR, SYNTHLINE, TOXCENTER, USAN, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

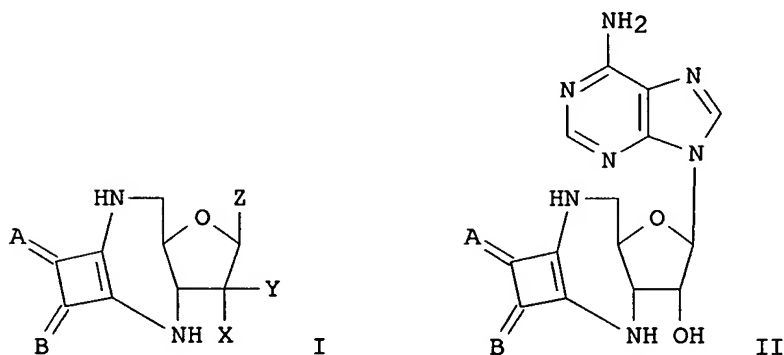
18 REFERENCES IN FILE CA (1907 TO DATE)
18 REFERENCES IN FILE CAPLUS (1907 TO DATE)

10/820,216

=> d ibib abs hitstr total

ANSWER 1 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2005:1003147 CAPLUS
 DOCUMENT NUMBER: 143:286635
 TITLE: Preparation of 3',5'-N,N'-(3,4-dioxocyclobutene-1,2-diyl)-3',5'-diamino-3',5'-dideoxynucleoside derivative as cyclic nucleotide analog
 INVENTOR(S): Sekine, Mitsuo; Seio, Yasushi; Miyashita, Takuhei
 PATENT ASSIGNEE(S): Japan Science and Technology Agency, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005247772	A2	20050915	JP 2004-61638	20040305
PRIORITY APPLN. INFO.:			JP 2004-61638	20040305
OTHER SOURCE(S):	CASREACT 143:286635; MARPAT 143:286635			
GI				



AB A 3',5'-diamino-3',5'-dideoxy-nucleoside derivative having squaric acid diamide skeleton (I) [A, B = O, S; one of X and Y = H and the other = H, halo, OH, NH₂, alkylamino, dialkylamino, alkoxy, alkoxyalkyl, aryloxyalkyl, arylthio, alkylthio, cyano, acylamino; Z = (un)substituted purin or pyrimidine base] is prepared This compound is relatively stable in vivo and exhibits resistance against degrading enzymes and is useful as an inhibitor or activator of intracellular or extracellular signal transduction (no data). Thus, 48 mg 3',5'-diamino-3',5'-dideoxyadenosine was dissolved in 1.5 mL MeOH, treated with 12.8 μL N,N-diisopropylethylamine and 17.1 mg 1,2-dimethoxy-3,4-dioxocyclobutene, and stirred at room temperature for 23 h to give, after purification by C-18 chromatog., 10 mg 3',5'-N,N'-(3,4-dioxocyclobutene-1,2-diyl)--3',5'-diamino-3',5'-dideoxyadenosine (II).

IT **864248-74-8P**
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

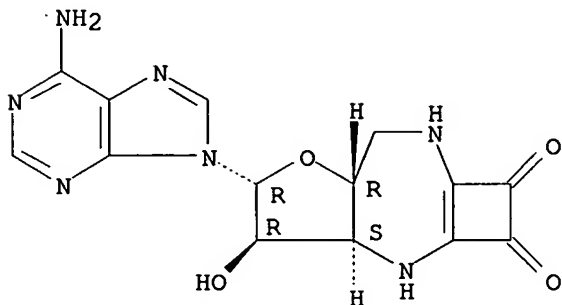
10/820,216

(preparation of 3',5'-N,N'-(3,4-dioxocyclobutene-1,2-diyl)-3',5'-diamino-3',5'-dideoxy-nucleoside derivative as cyclic nucleotide analog and cellular signal transduction activator or inhibitor)

RN 864248-74-8 CAPLUS

CN 2H-Cyclobuta[b]furo[3,2-e][1,4]diazepine-5,6-dione, 2-(6-amino-9H-purin-9-yl)-3,3a,4,7,8,8a-hexahydro-3-hydroxy-, (2R,3R,3aS,8aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



applied

L11 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2005:572349 CAPLUS
 DOCUMENT NUMBER: 143:103227
 TITLE: Oral administration of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)alkyl] phosphonic acid and derivatives
 INVENTOR(S): Benjamin, Eric J.; Cloud, William F.; Ashraf, Muhammad; Islam, Mohammed; Brandt, Michael R.; Tremblay, Gerald F.
 PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
 SOURCE: U.S. Pat. Appl. Publ., 32 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 4
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005142192	A1	20050630	US 2004-961871	20041008
US 2005004079	A1	20050106	US 2004-820215	20040407
US 2005004080	A1	20050106	US 2004-820216	20040407
PRIORITY APPLN. INFO.:			US 2003-511560P	P 20031015
			US 2004-820215	A 20040407
			US 2004-820216	A 20040407
			US 2003-461490P	P 20030409
			US 2003-461571P	P 20030409

OTHER SOURCE(S): MARPAT 143:103227

AB Solid, pharmaceutical dosage forms of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)alkyl]phosphonic acid and derivs. thereof are disclosed. In addition, methods of use are disclosed for the treatment, inter alia, of cerebral vascular disorders, anxiety disorders; mood disorders; schizophrenia; schizophreniform disorder; schizoaffective disorder; cognitive impairment; chronic neurodegenerative disorders; inflammatory diseases; fibromyalgia; complications from herpes zoster; prevention of tolerance to opiate analgesia; withdrawal symptoms from addictive drugs; and pain. For example, enteric coated tablets contained [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl] phosphonic acid 200, croscarmellose sodium 7.05, Povidone 3.53, Avicel PH101 14.1, croscarmellose sodium 4.7, sodium lauryl sulfate 5.88 and magnesium stearate 1.18 mg.

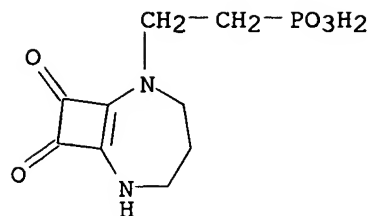
IT 144912-63-0 780765-59-5 780765-64-2
 780765-66-4 780765-67-5 782452-07-7
 782452-08-8 782452-09-9 782452-10-2
 782452-11-3

RL: PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(oral administration of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)alkyl] phosphonic acid and derivs. for the treatment of mental disorders and inflammatory diseases and pain relief)

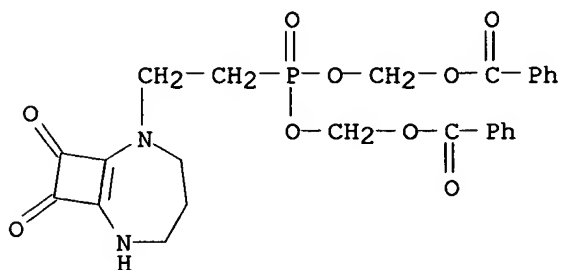
RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



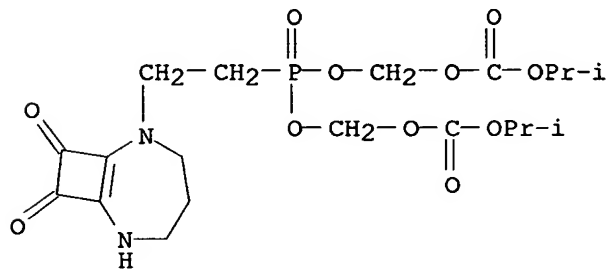
RN 780765-59-5 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[(benzoyloxy)methyl] ester (9CI) (CA INDEX NAME)



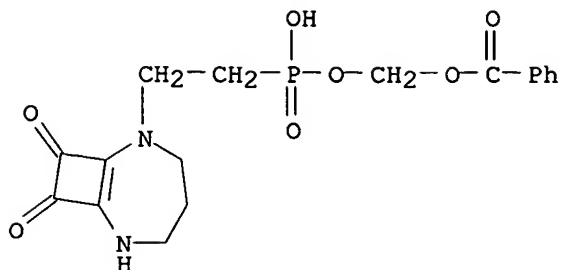
RN 780765-64-2 CAPLUS

CN 2,4,6,8-Tetraoxa-5-phosphanonanedioic acid, 5-[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis(1-methylethyl) ester, 5-oxide (9CI) (CA INDEX NAME)



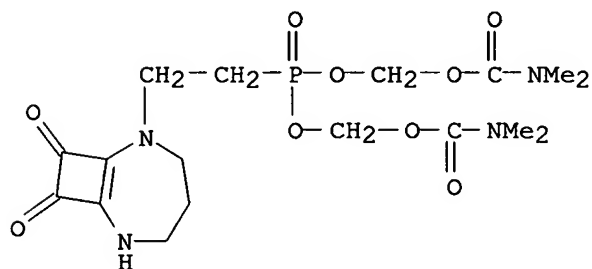
RN 780765-66-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, mono[(benzoyloxy)methyl] ester (9CI) (CA INDEX NAME)



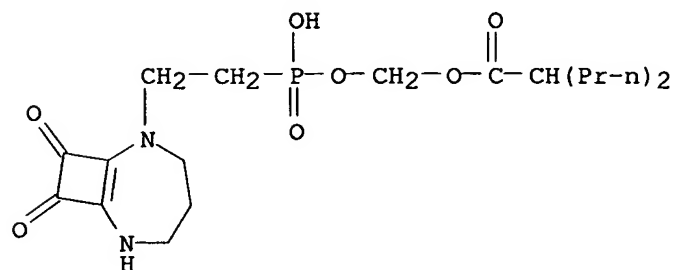
RN 780765-67-5 CAPLUS

CN Carbamic acid, dimethyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxyethylene) ester (9CI) (CA INDEX NAME)



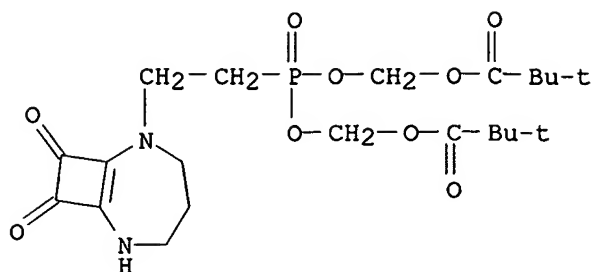
RN 782452-07-7 CAPLUS

CN Pentanoic acid, 2-propyl-, [[[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]hydroxyphosphinyl]oxy]methyl ester (9CI) (CA INDEX NAME)



RN 782452-08-8 CAPLUS

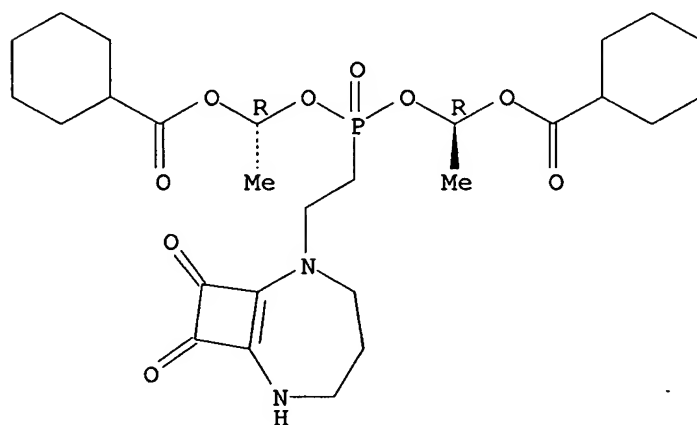
CN Propanoic acid, 2,2-dimethyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxyethylene) ester (9CI) (CA INDEX NAME)



RN 782452-09-9 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis[oxy-(1R)-ethylidene] ester (9CI) (CA INDEX NAME)

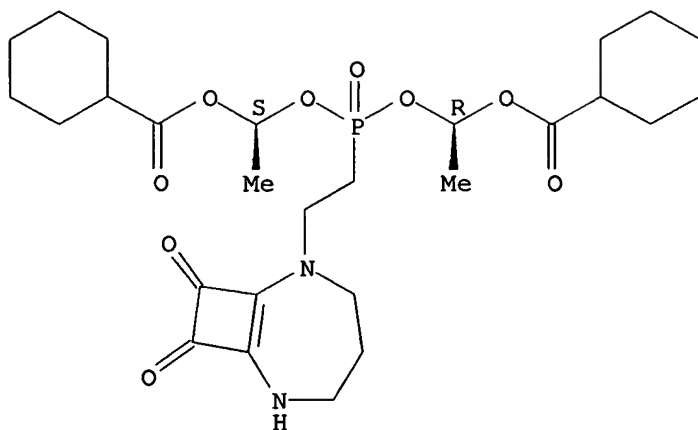
Relative stereochemistry.



RN 782452-10-2 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxyethylidene) ester, stereoisomer (9CI) (CA INDEX NAME)

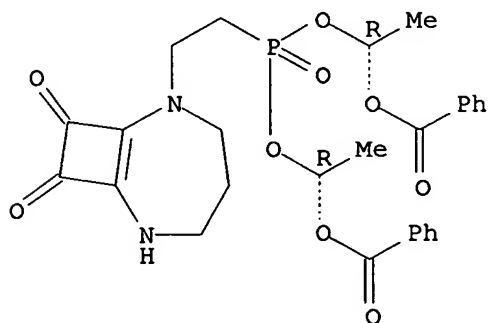
Relative stereochemistry.



RN 782452-11-3 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[(1R)-1-(benzyloxymethyl)ethyl] ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L11 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:371071 CAPLUS

DOCUMENT NUMBER: 142:417206

TITLE: Oral administration of NMDA receptor antagonists

INVENTOR(S): Benjamin, Eric J.; Cloud, William F.; Ashraf, Muhammad; Islam, Mohammed; Brandt, Michael R.; Tremblay, Gerald F.

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037287	A1	20050428	WO 2004-US34113	20041014
WO 2005037287	C1	20050630		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: US 2003-511560P P 20031015

OTHER SOURCE(S): MARPAT 142:417206

AB Solid, oral pharmaceutical dosage forms of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)alkyl]phosphonic acid and its derivs. (salts) as NMDA receptor antagonists are disclosed. In addition, methods of use are disclosed for the treatment, inter alia, of cerebral vascular disorders, anxiety disorders; mood disorders; schizophrenia; schizophreniform disorder; schizoaffective disorder; cognitive impairment; chronic neurodegenerative disorders; inflammatory diseases; fibromyalgia; complications from herpes zoster; prevention of tolerance to opiate analgesia; withdrawal symptoms from addictive drugs; and pain. For example, a capsule formulation was prepared by wet granulation comprising (i) an intragranular phase containing [2-[8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl]ethyl]phosphonic acid 100 mg, Avicel PH 101 13.91 mg, povidone 3.61 mg, and croscarmellose sodium 5.77 mg, and (ii) an extragranular phase containing Avicel PH 101 14.42 mg, croscarmellose sodium 5.77 mg, and magnesium stearate 1.44 mg.

IT 144912-63-0

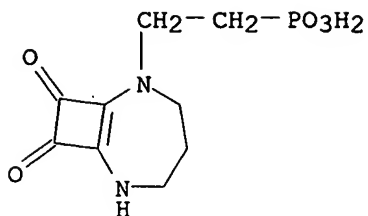
RL: PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation, bioavailability and therapeutic uses of oral compns. containing

phosphonate derivs. as NMDA antagonists)

RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



IT 780765-59-5 780765-62-0 780765-63-1
 780765-64-2 780765-66-4 780765-67-5
 780765-68-6 782452-08-8 850148-47-9

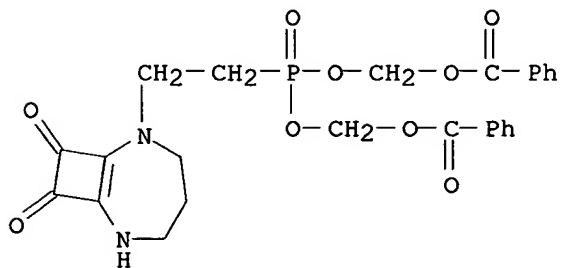
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
 (preparation, bioavailability and therapeutic uses of oral compns.

containing

phosphonate derivs. as NMDA antagonists)

RN 780765-59-5 CAPLUS

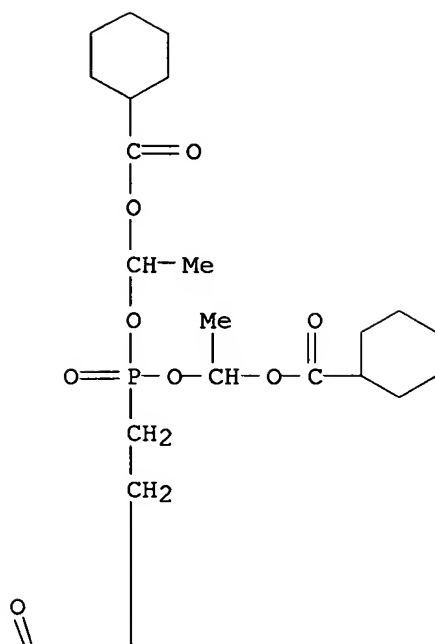
CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[(benzoyloxy)methyl] ester (9CI) (CA INDEX NAME)



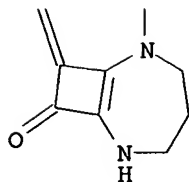
RN 780765-62-0 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-6-yl)ethyl]phosphinylidene]bis(oxyethylidene) ester (9CI) (CA INDEX NAME)

PAGE 1-A

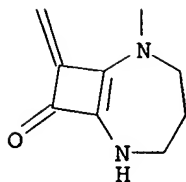
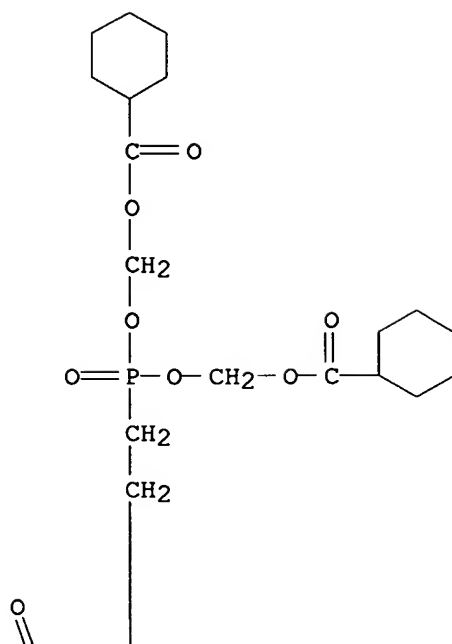


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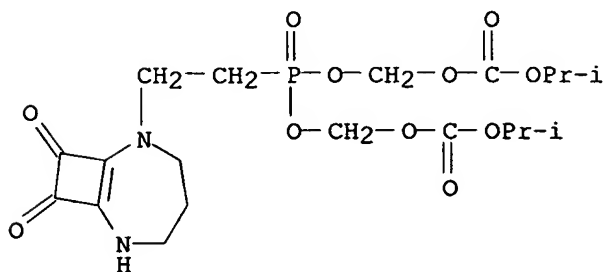
RN 780765-63-1 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-6-yl)ethyl]phosphinylidene]bis(oxymethylene) ester (9CI) (CA INDEX NAME)



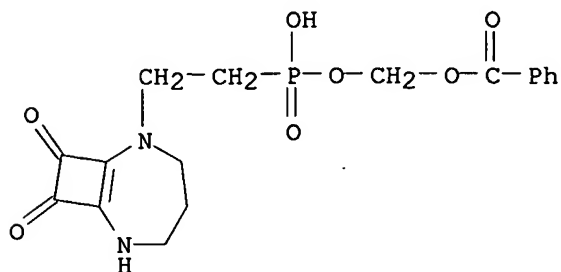
RN 780765-64-2 CAPLUS

CN 2,4,6,8-Tetraoxa-5-phosphanonanedioic acid, 5-[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis(1-methylethyl) ester, 5-oxide (9CI) (CA INDEX NAME)



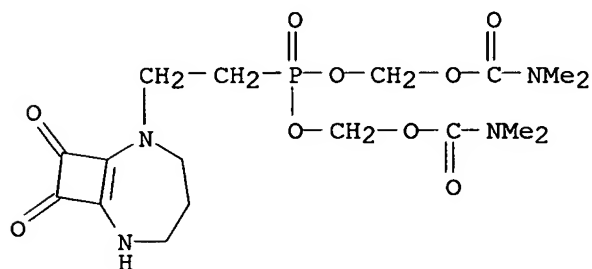
RN 780765-66-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, mono[(benzyloxy)methyl] ester (9CI) (CA INDEX NAME)



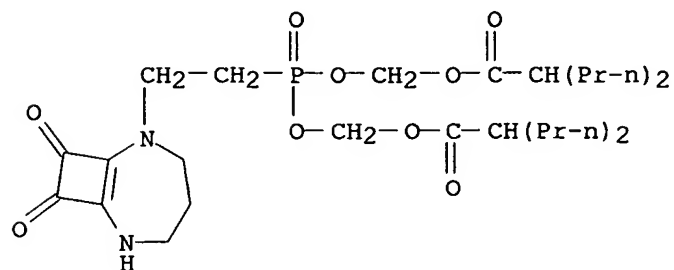
RN 780765-67-5 CAPLUS

CN Carbamic acid, dimethyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxymethylene) ester (9CI) (CA INDEX NAME)



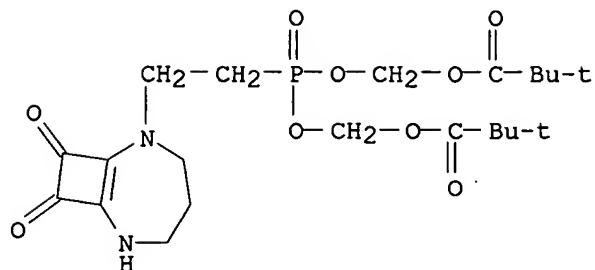
RN 780765-68-6 CAPLUS

CN Pentanoic acid, 2-propyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxymethylene) ester (9CI) (CA INDEX NAME)



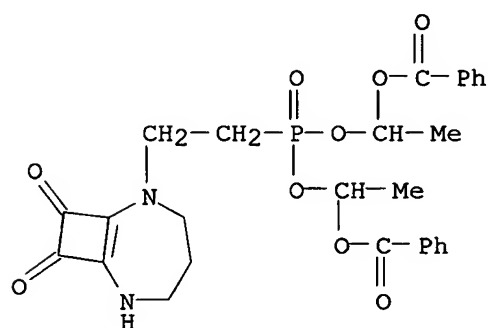
RN 782452-08-8 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxymethylene) ester (9CI) (CA INDEX NAME)



RN 850148-47-9 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[1-(benzoyloxy)ethyl] ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

2

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

111 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:371019 CAPLUS

DOCUMENT NUMBER: 142:411486

TITLE: Preparation of {2-[8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl]ethyl}phosphonate esters by cyclocondensation reaction of squaric acid derivatives with (aminopropyl)aminoethanephosphonate esters and subsequent hydrolysis to free acid

INVENTOR(S): Wilk, Bogdan K.; Vid, Galina; Liu, Weiguo; Shi, Xinxu

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: U.S. Pat. Appl. Publ., 10 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005090470	A1	20050428	US 2004-969715	20041020
WO 2005040176	A2	20050506	WO 2004-US34831	20041020
WO 2005040176	A3	20051201		

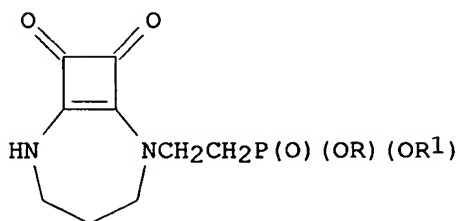
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

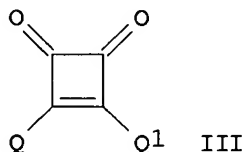
PRIORITY APPLN. INFO.: US 2003-513611P P 20031022

OTHER SOURCE(S): CASREACT 142:411486; MARPAT 142:411486

GI



I



III

AB {2-[8,9-Dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl]ethyl}phosphonic acid (I; R = R1 = H), useful as an NMDA antagonist appropriate for treatment of stroke, epilepsy, Alzheimer's and Parkinson's diseases and pain (no data), is prepared by hydrolysis of its esters I (R, R1 = C1-6 alkyl, C1-6 haloalkyl; preferably R = R1 = Et), which in turn are prepared by reaction of a 1,3-diaminopropane derivative H2N(CH2)3NHCH2CH2P(O)(OR)(OR1) (II; same R, R1) with a cyclobutenedione (III; Q, Q1 = OH, halo, OX1;

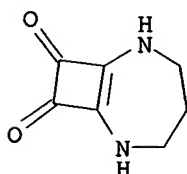
preferably Q, Q1 = OEt or OH; X1 = C1-6 alkyl, C1-6 haloalkyl, aryl) in a solvent HOX1 (same X1; preferably HOX1 = MeOH or EtOH); compds. II are prepared by reaction of 1,3-diaminopropane with XCH₂CH₂P(O)(OR)(OR1) or CH₂:CHP(O)(OR)(OR1) (same R, R1; X = leaving group, preferably halo) at a ratio of ≥2:1. In an example, treating 1.04 g di-Et squarate III (Q = Q1 = OEt) in 250 mL MeOH with 1.46 g II (R = R1 = Et; preparation given.) in 50 mL MeOH at 60° for 6 h and subsequent stirring overnight at room temperature gave 54% title ester I (R = R1 = Et).

IT **66086-41-7P**

RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
(preparation of [[dioxodiazabicyclo[5.2.0]nonenyl]ethyl]phosphonates by cyclocondensation reaction of squaric acid derivs. with diaminopropane phosphonate derivs. and hydrolysis to give free acid)

RN 66086-41-7 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione (9CI) (CA INDEX NAME)



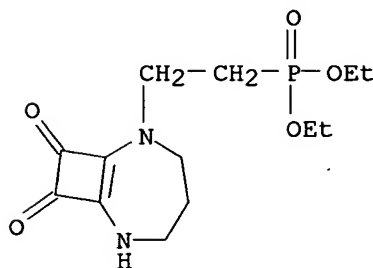
IT **144912-83-4P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [[dioxodiazabicyclo[5.2.0]nonenyl]ethyl]phosphonates by cyclocondensation reaction of squaric acid derivs. with diaminopropane phosphonate derivs. and hydrolysis to give free acid)

RN 144912-83-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



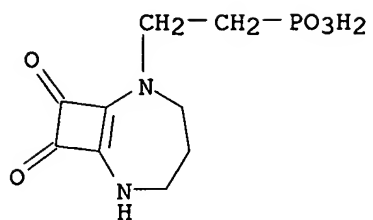
IT **144912-63-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [[dioxodiazabicyclo[5.2.0]nonenyl]ethyl]phosphonates by cyclocondensation reaction of squaric acid derivs. with diaminopropane phosphonate derivs. and hydrolysis to give free acid)

RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)

10/820,216

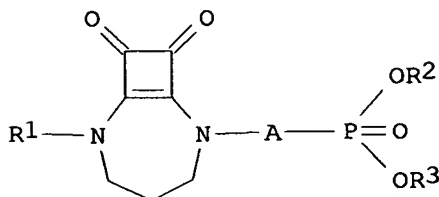


10/820,216

applicant

L11 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:902398 CAPLUS
DOCUMENT NUMBER: 141:380023
TITLE: Preparation of derivatives of 2-(8,9-dioxo-2,6-diazabicyclo(5.2.0)non-1(7)-en-2-yl)alkylphosphonic acid and their use as n-methyl-d-aspartate (nmda) receptor antagonists
INVENTOR(S): Baudy, Reinhardt Bernhard; Butera, John Anthony
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092189	A1	20041028	WO 2004-US10596	20040407
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2521313	AA	20041028	CA 2004-2521313	20040407
EP 1611144	A1	20060104	EP 2004-759168	20040407
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
PRIORITY APPLN. INFO.:			US 2003-461490P	P 20030409
			WO 2004-US10596	W 20040407
OTHER SOURCE(S):			CASREACT 141:380023; MARPAT 141:380023	
GI				



I

AB Preparation of title compds. I (at least one R2 or R3 is not hydrogen; R1 = H, C1-6 alkyl, C2-7 acyl, C1-6 alkanesulfonyl, C6-14 aroyl; R2, R3 = H, (un)substituted alkylcarboxyalkyl, alkoxyalkyl, aminocarboxyalkyl; A = C1-4 alkylene, C2-4 alkenylene) or pharmaceutically acceptable salts

thereof are provided. The compds. of the present invention are N-methyl-D-aspartate (NMDA) receptor antagonists and are useful in treating a variety of conditions present in a mammal that benefit from inhibiting the NMDA receptor. Thus, reaction of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid with benzoic acid chloromethyl ester in DMF in the presence of N,N-diisopropylethylamine gave 99% title compound, 3-(2-[8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl)-3-oxido-7-oxo-7-phenyl-2,4,6-trioxa-3-phosphahept-1-yl benzoate.

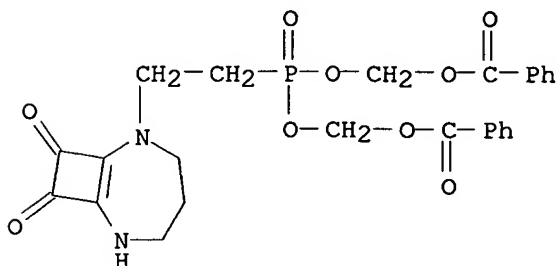
IT **780765-59-5P**

RL: BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of derivs. of dioxodiazabicyclononenalkylphosphonic acid and their use as Me aspartate NMDA receptor antagonists)

RN 780765-59-5 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[(benzoyloxy)methyl] ester (9CI) (CA INDEX NAME)



IT **780765-63-1P 780765-64-2P 780765-66-4P**

780765-67-5P 782452-07-7P 782452-08-8P

782452-09-9P 782452-10-2P 782452-11-3P

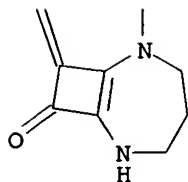
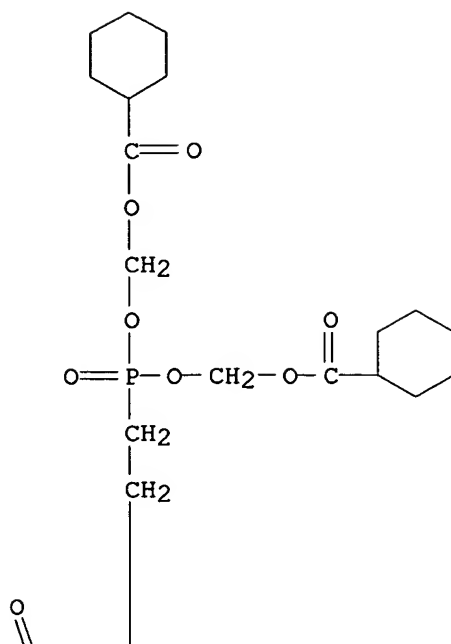
782452-12-4P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of derivs. of dioxodiazabicyclononenalkylphosphonic acid and their use as Me aspartate NMDA receptor antagonists)

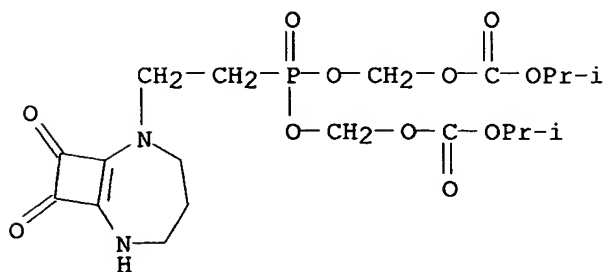
RN 780765-63-1 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-6-yl)ethyl]phosphinylidene]bis(oxyethylene) ester (9CI) (CA INDEX NAME)



RN 780765-64-2 CAPLUS

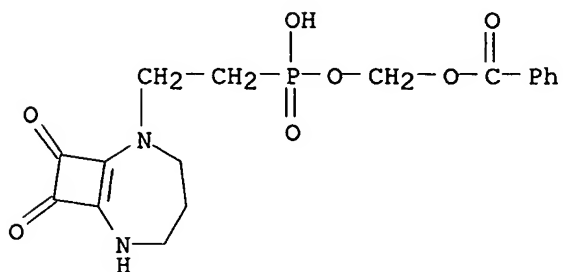
CN 2,4,6,8-Tetraoxa-5-phosphanonanedioic acid, 5-[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis(1-methylethyl) ester, 5-oxide (9CI) (CA INDEX NAME)



10/820,216

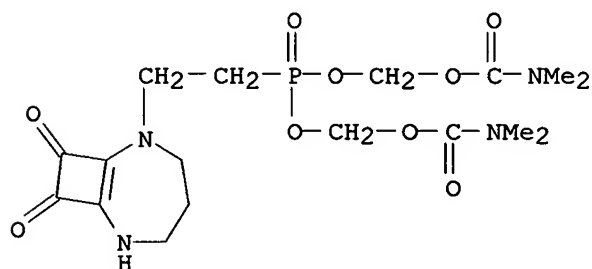
RN 780765-66-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, mono[(benzoyloxy)methyl] ester (9CI) (CA INDEX NAME)



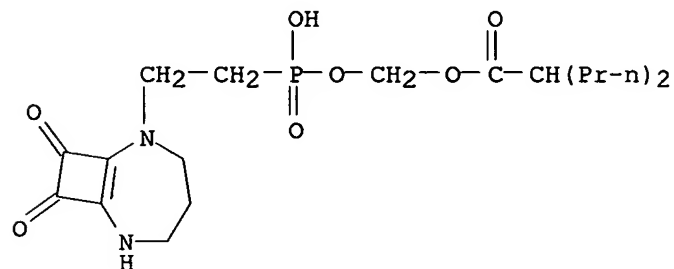
RN 780765-67-5 CAPLUS

CN Carbamic acid, dimethyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxyethylene) ester (9CI) (CA INDEX NAME)



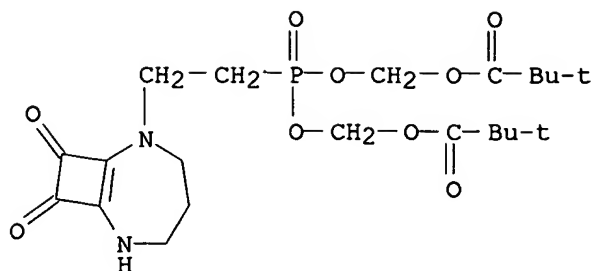
RN 782452-07-7 CAPLUS

CN Pentanoic acid, 2-propyl-, [[[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]hydroxyphosphinyl]oxy]methyl ester (9CI) (CA INDEX NAME)



RN 782452-08-8 CAPLUS

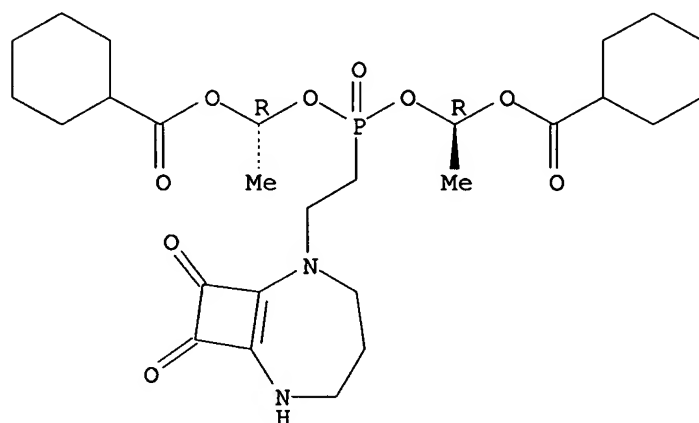
CN Propanoic acid, 2,2-dimethyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxyethylene) ester (9CI) (CA INDEX NAME)



RN 782452-09-9 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis[oxy-(1R)-ethylidene] ester (9CI) (CA INDEX NAME)

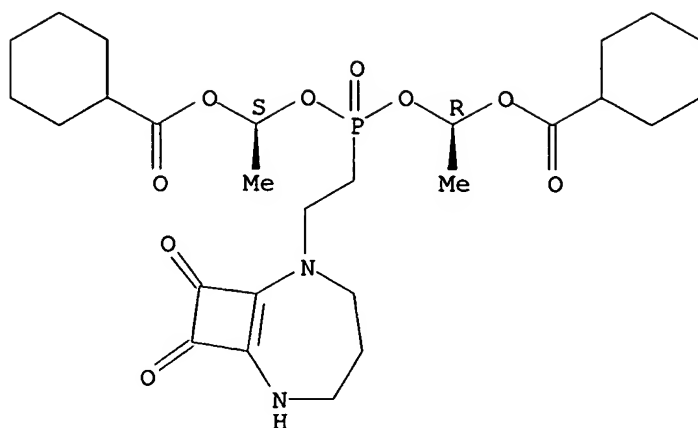
Relative stereochemistry.



RN 782452-10-2 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxyethylidene) ester, stereoisomer (9CI) (CA INDEX NAME)

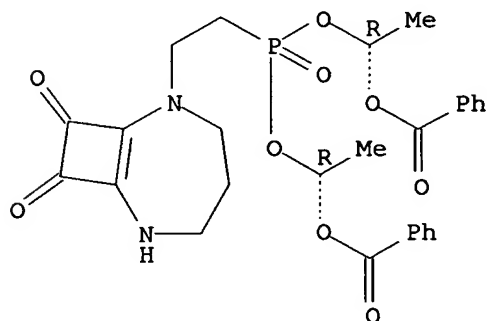
Relative stereochemistry.



RN 782452-11-3 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[(1R)-1-(benzoyloxy)ethyl] ester, rel- (9CI) (CA INDEX NAME)

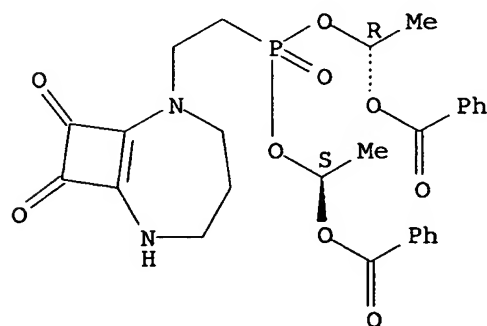
Relative stereochemistry.



RN 782452-12-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, (1R)-1-(benzoyloxy)ethyl (1S)-1-(benzoyloxy)ethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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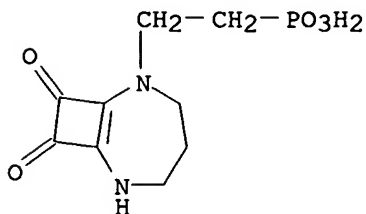
IT 144912-63-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of derivs. of dioxodiazabicyclononenalkylphosphonic acid and their use as Me aspartate NMDA receptor antagonists)

RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

22

THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:902198 CAPLUS

DOCUMENT NUMBER: 141:370576

TITLE: Intranasal pharmaceutical compositions containing
[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)alkyl]phosphonic acid and its derivativesINVENTOR(S): Benjamin, Eric Joel; Baudy, Reinhardt Bernhard;
Brandt, Michael Richard

PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA

SOURCE: PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091633	A1	20041028	WO 2004-US11668	20040407
WO 2004091633	C1	20050113		
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RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2521394	AA	20041028	CA 2004-2521394	20040407
EP 1622625	A1	20060208	EP 2004-759562	20040407
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR			
PRIORITY APPLN. INFO.:			US 2003-461571P	P 20030409
			WO 2004-US11668	W 20040407

OTHER SOURCE(S): MARPAT 141:370576

AB Pharmaceutical compns. for intranasal administration contain the title compound or a salt thereof, and 1 or more additives for forming a composition for

intranasal administration. Also provided are methods of treating conditions in a mammal associated with a glutamate abnormality that includes administering intranasally to a mammal a therapeutically effective amount of the above compds. Thus, a nasal solution contained [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid 30.0 and EDTA 0.10 g, 5N NaOH solution 37 and water 50 mL.

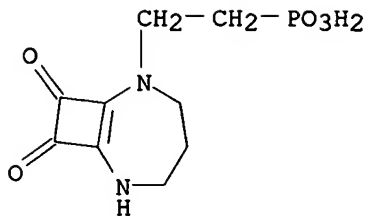
IT 144912-63-0

RL: PKT (Pharmacokinetics); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(intranasal pharmaceutical compns. containing dioxo(diazabicyclononyl)alkylphosphonic acid and its derivs.)

RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)

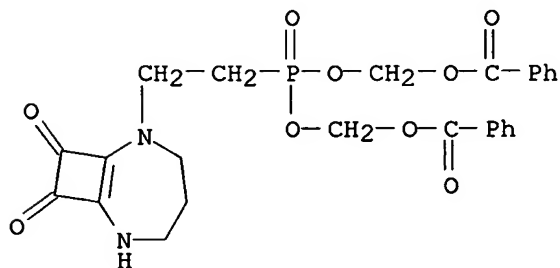


IT 780765-59-5P

RL: PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(intranasal pharmaceutical comps. containing dioxo(diazabicyclononyl)alkylphosphonic acid and its derivs.)

RN 780765-59-5 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[(benzoyloxy)methyl] ester (9CI) (CA INDEX NAME)



IT 780765-60-8 780765-61-9 780765-62-0

780765-63-1 780765-64-2 780765-65-3

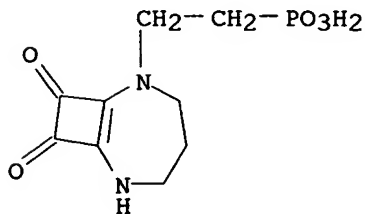
780765-66-4 780765-67-5 780765-68-6

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(intranasal pharmaceutical comps. containing dioxo(diazabicyclononyl)alkylphosphonic acid and its derivs.)

RN 780765-60-8 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, sodium salt (9CI) (CA INDEX NAME)

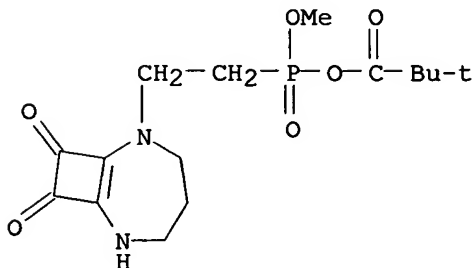


● x Na

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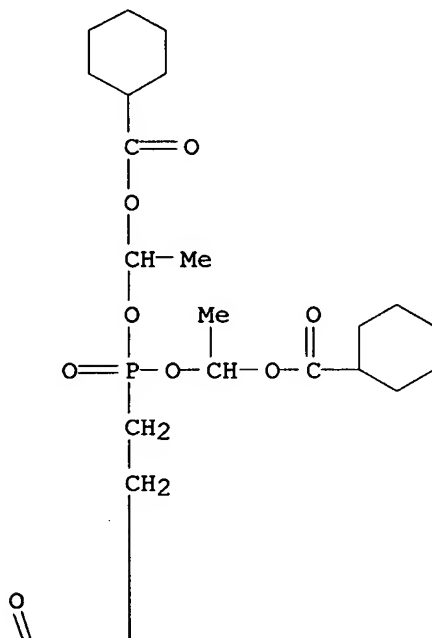
RN 780765-61-9 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, anhydride with methyl hydrogen
[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonate
(9CI) (CA INDEX NAME)



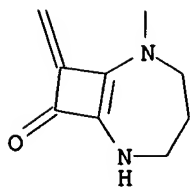
RN 780765-62-0 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-
en-6-yl)ethyl]phosphinylidene]bis(oxyethylidene) ester (9CI) (CA INDEX
NAME)



PAGE 1-A

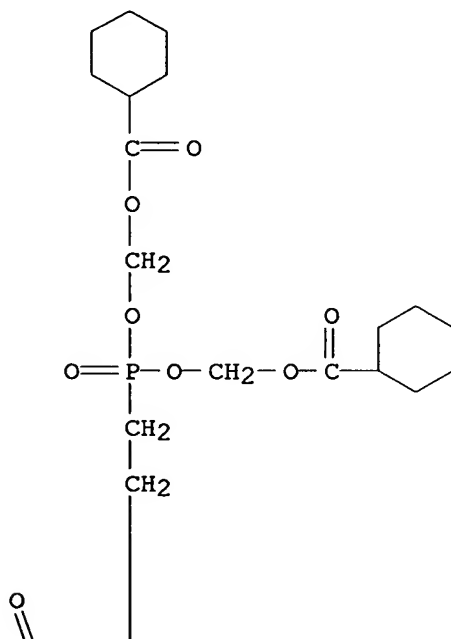
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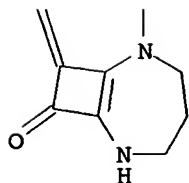
RN 780765-63-1 CAPLUS

CN Cyclohexanecarboxylic acid, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-6-yl)ethyl]phosphinylidene]bis(oxyethylene) ester (9CI) (CA INDEX NAME)

PAGE 1-A



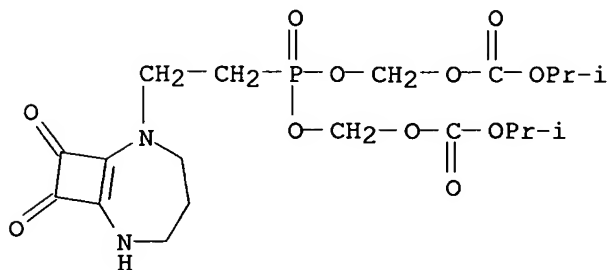
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RN 780765-64-2 CAPLUS

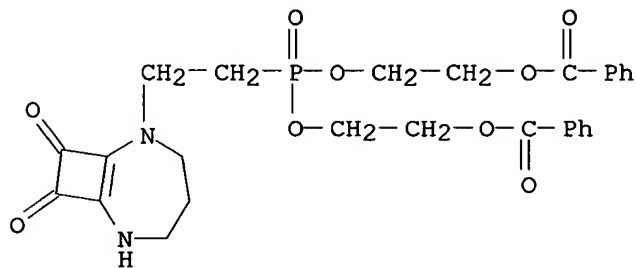
CN 2,4,6,8-Tetraoxa-5-phosphanonanedioic acid, 5-[2-(8,9-dioxo-2,6-

diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis(1-methylethyl) ester, 5-oxide (9CI) (CA INDEX NAME)



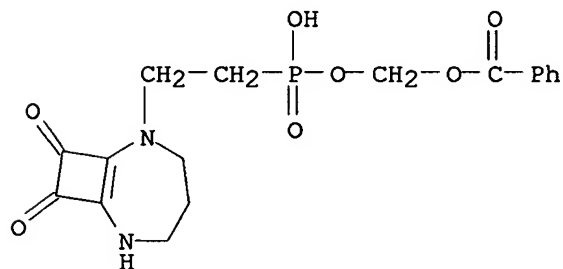
RN 780765-65-3 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, bis[2-(benzoyloxy)ethyl] ester (9CI) (CA INDEX NAME)



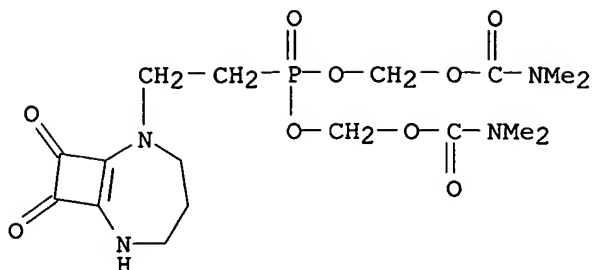
RN 780765-66-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, mono[(benzoyloxy)methyl] ester (9CI) (CA INDEX NAME)



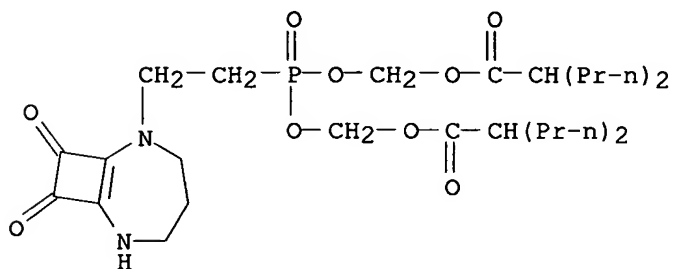
RN 780765-67-5 CAPLUS

CN Carbamic acid, dimethyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinyldiene]bis(oxymethylene) ester (9CI) (CA INDEX NAME)



RN 780765-68-6 CAPLUS

CN Pentanoic acid, 2-propyl-, [[2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphinylidene]bis(oxymethylene) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

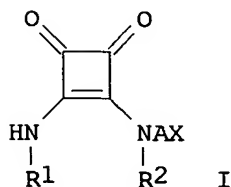
4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/820,216

~~1~~1 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:301059 CAPLUS
DOCUMENT NUMBER: 138:314606
TITLE: [[2-(amino-3,4-dioxo-1-cyclobuten-1-yl)amino]alkyl]-
acid derivatives for the treatment of pain
INVENTOR(S): Brandt, Michael Richard; Zaleska, Margaret Maria;
Moyer, John Allen
PATENT ASSIGNEE(S): Wyeth, John, and Brother Ltd., USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003031416	A2	20030417	WO 2002-US32252	20021009
WO 2003031416	A3	20030814		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2461348	AA	20030417	CA 2002-2461348	20021009
US 2003114444	A1	20030619	US 2002-267159	20021009
EP 1434588	A2	20040707	EP 2002-789180	20021009
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
BR 2002013237	A	20040928	BR 2002-13237	20021009
JP 2005508950	T2	20050407	JP 2003-534400	20021009
NO 2004001378	A	20040528	NO 2004-1378	20040402
PRIORITY APPLN. INFO.:			US 2001-328245P	P 20011010
			WO 2002-US32252	W 20021009
OTHER SOURCE(S):	MARPAT 138:314606			
GI				



AB The invention provides a method for treating pain in a mammal that includes administering I [R1 = H, C1-6 alkyl, C7-12 phenylalkyl; R2 = H, C1-6 alkyl, C2-6 alkenyl, C7-12 phenylalkyl; or R1 and R2 taken together

as Z are CH₂CH₂, CH₂C(R₆)(R₇)CH₂, CH₂C(R₈)(R₉)C(R₁₀)(R₁₁)CH₂; R₆, R₈, R₁₀ = H, C1-6 alkyl, OH; R₇, R₉, R₁₁ = H, C1-6 alkyl; A = C1-6 alkylene, C2-6 alkenylene; X = CO₂R₃, P(O)(OR₄)(OR₅), 3,5-dioxo-1,2,4-oxadiazolidin-2-yl, 5-tetrazolyl; R₃, R₄, R₅ = H, C1-6 alkyl], or a pharmaceutically acceptable salt thereof. Also provided are compns. for treating pain containing I.

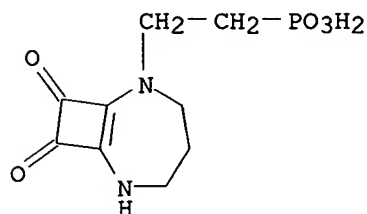
IT 144912-63-0 144912-64-1 144912-67-4

144912-69-6

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(aminodioxocyclobutenyl derivs. for treatment of pain)

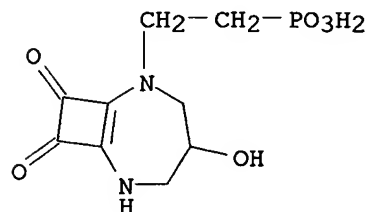
RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



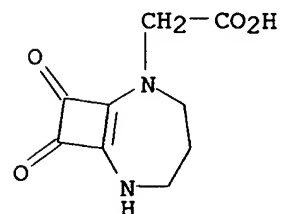
RN 144912-64-1 CAPLUS

CN Phosphonic acid, [2-(4-hydroxy-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 144912-67-4 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetic acid, 8,9-dioxo- (9CI) (CA INDEX NAME)

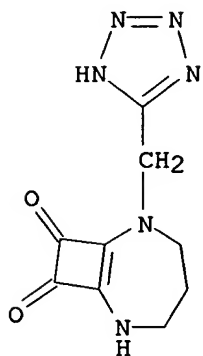


RN 144912-69-6 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione, 2-(1H-tetrazol-5-ylmethyl)-

10/820,216

(9CI) (CA INDEX NAME)



10/820,216

LM ANSWER 8 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:748347 CAPLUS

DOCUMENT NUMBER: 131:337040

TITLE: Preparation of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid

INVENTOR(S): Asselin, Andre A.; Kinney, William A.; Schmid, Jean

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: U.S., 6 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5990307	A	19991123	US 1998-127202	19980731
US 6011168	A	20000104	US 1999-375345	19990816
PRIORITY APPLN. INFO.:			US 1997-54553P	P 19970801
			US 1998-127202	A3 19980731

OTHER SOURCE(S): CASREACT 131:337040

AB [2-(8,9-Dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid (I) was prepared by reaction of Me₃CO₂CNH(CH₂)₃NH₂ with a dialkyl vinylphosphonate to obtain N-[3-(t-butyloxycarbonylamino)propyl]-2-aminoethylphosphonic acid dialkyl ester in 80% yield. Reaction of the latter with a 3,4-dialkoxycyclobut-3-en-1,2-dione gave [3-[[2-(dialkoxyphosphoryl)ethyl]-(2-alkoxy-3,4-dioxo-1,2-cyclobuten-1-yl)amino]propyl]carbamic acid 1,1-dimethylethyl ester in 96% yield. Deprotection and cyclization of this in CF₃CO₂H gave [2-((8,9)-dioxo-2,6-diazabicyclo[5.2.0]-non-1(7)-en-2-yl)ethyl]phosphonic acid dialkyl ester in 58% yield; treatment with BrSiMe₃ gave I in 38.8% overall yield.

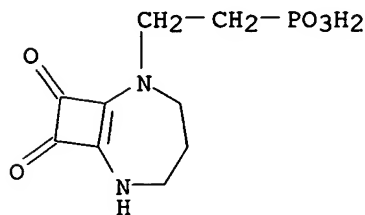
IT **144912-63-0P**

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid)

RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



IT **144912-83-4P**

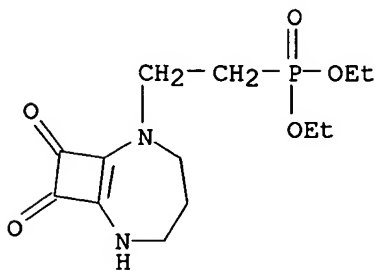
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid)

RN 144912-83-4 CAPLUS

10/820,216

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

111 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:113692 CAPLUS

DOCUMENT NUMBER: 130:153793

TITLE: Preparation of [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid

INVENTOR(S): Asselin, Andre Alfred; Kinney, William Alvin; Schmid, Jean

PATENT ASSIGNEE(S): American Home Products Corporation, USA

SOURCE: PCT Int. Appl., 17 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906417	A1	19990211	WO 1998-US15841	19980731
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2297411	AA	19990211	CA 1998-2297411	19980731
AU 9886037	A1	19990222	AU 1998-86037	19980731
AU 746119	B2	20020418		
EP 1000072	A1	20000517	EP 1998-937292	19980731
EP 1000072	B1	20030219		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
BR 9811807	A	20000815	BR 1998-11807	19980731
JP 2001512129	T2	20010821	JP 2000-505174	19980731
NZ 502509	A	20020828	NZ 1998-502509	19980731
AT 232875	E	20030315	AT 1998-937292	19980731
RU 2205834	C2	20030610	RU 2000-105273	19980731
ES 2190091	T3	20030716	ES 1998-937292	19980731
CN 1526714	A	20040908	CN 2003-10120120	19980731
NO 2000000488	A	20000131	NO 2000-488	20000131
HK 1027814	A1	20030516	HK 2000-107097	20001108
PRIORITY APPLN. INFO.:			US 1997-905091	A 19970801
			WO 1998-US15841	W 19980731

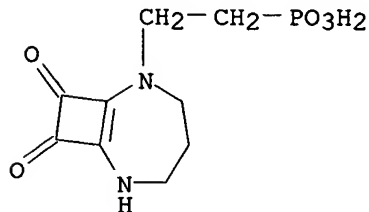
AB The title compound (I), an NMDA antagonist, was useful as an anticonvulsant and neuroprotectant in situations involving excess release of excitatory amino acids. 3-Aminopropylcarbamic acid 1,1-dimethyl-Et ester was treated with a dialkyl vinylphosphonate (alkyl = Me, Et) to obtain N-[3-(tert-butyloxycarbonylamino)propyl]-2-aminoethylphosphonic acid dialkyl ester (II) in 80% yield. Reaction of II with 3,4-diethoxycyclobut-3-ene-1,2-dione gave [3-[[2-(dialkoxyphosphoryl)ethyl]-(2-alkoxy-3,4-dioxo-1,2-cyclobuten-1-yl)amino]propyl]carbamic acid 1,1-dimethylethyl ester (III) in 96% yield. Deprotection and cyclization of III in HO₂CCF₃ gives [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid dialkyl ester (IV) in 58% yield. Compound IV was treated with bromotrimethylsilane to give I.

IT 144912-63-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)

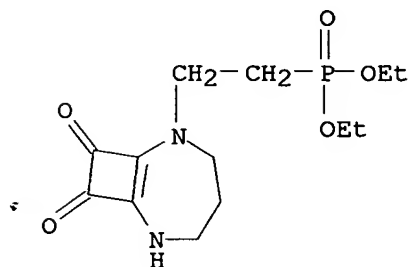


IT 144912-83-4P 220288-14-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of [(dioxodiazabicyclo[5.2.0]nonenyl)ethyl]phosphonic acid
esters)

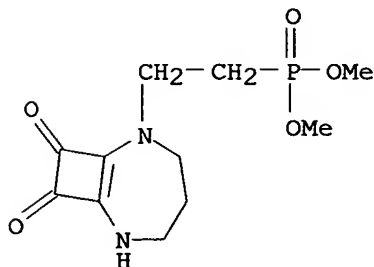
RN 144912-83-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 220288-14-2 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, dimethyl ester (9CI) (CA INDEX NAME)



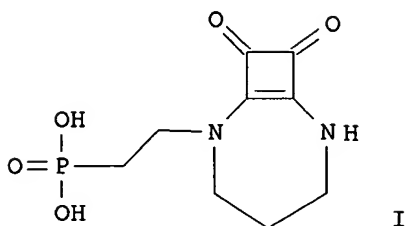
REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/820,216

111 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1998:9157 CAPLUS
 DOCUMENT NUMBER: 128:75452
 TITLE: Design and Synthesis of [2-(8,9-Dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic Acid (EAA-090), a Potent N-Methyl-D-aspartate Antagonist, via the Use of 3-Cyclobutene-1,2-dione as an Achiral α -Amino Acid Bioisostere
 AUTHOR(S): Kinney, William A.; Abou-Gharbia, Magid; Garrison, Deanna T.; Schmid, Jean; Kowal, Dianne M.; Bramlett, Donna R.; Miller, Tracy L.; Tasse, Rene P.; Zaleska, Margaret M.; Moyer, John A.
 CORPORATE SOURCE: Chemical Sciences CNS Disorders Divisions, Wyeth-Ayerst Research, Princeton, NJ, 08543-8000, USA
 SOURCE: Journal of Medicinal Chemistry (1998), 41(2), 236-246
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 128:75452
 GI



- AB The diazabicyclic amino acid phosphonate I, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid, was identified as a potent NMDA antagonist. It contains the α -amino acid bioisostere 3,4-diamino-3-cyclobutene-1,2-dione and an addnl. ring for conformational rigidity. I was as potent as CGS-19755 in the [3H]CPP binding assay, the stimulated [3H]TCP binding assay, and the NMDA-induced lethality model in mice. A single bolus dose of I, administered i.v. following permanent occlusion of middle cerebral artery (MCA) in the rat, reduced the size of infarcted tissue by 57%. Structure-activity relationship (SAR) studies have indicated that the six- and eight-membered ring derivs. had diminished activity and that the two-carbon side chain length was optimum for NMDA receptor affinity. Substitution on the ring was counterproductive in the case of sterically demanding di-Me groups and of no consequence in the case of an H-bonding hydroxyl group. Replacement of the phosphonic acid group by either a carboxylic acid or a tetrazole group was unproductive. The potent bicyclic NMDA antagonists were synthesized efficiently by virtue of their achiral nature and the ease of vinylogous amide formation from squaric acid esters. I, being a unique NMDA antagonist structural type with a favorable preclin. profile, may offer advantages over existing NMDA antagonists for the treatment of neurol. disorders such as stroke and head trauma. I is currently under clin. evaluation as a neuroprotective agent for stroke.
- IT 144912-54-9P 144912-55-0P 144912-64-1P
 144912-65-2P 144912-66-3P 144912-69-6P

144913-00-8P 144913-01-9P

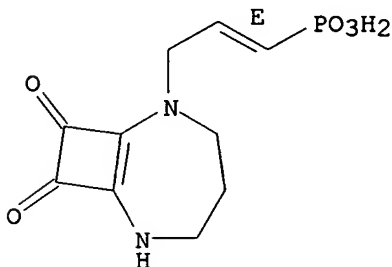
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(design and synthesis of [(dioxodiazabicyclononyl)ethyl]phosphonic acid as a potent NMDA antagonist via use of cyclobutenedione as achiral amino acid bioisostere)

RN 144912-54-9 CAPLUS

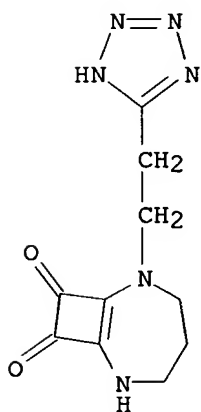
CN Phosphonic acid, [3-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)-1-propenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



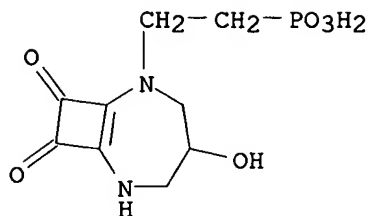
RN 144912-55-0 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione, 2-[2-(1H-tetrazol-5-yl)ethyl]- (9CI) (CA INDEX NAME)



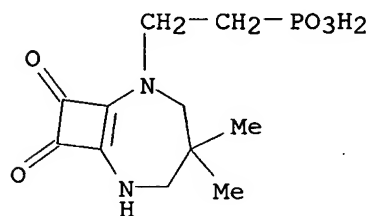
RN 144912-64-1 CAPLUS

CN Phosphonic acid, [2-(4-hydroxy-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



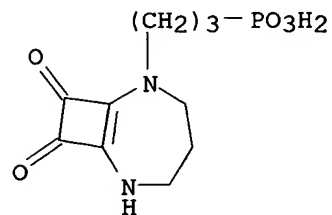
RN 144912-65-2 CAPLUS

CN Phosphonic acid, [2-(4,4-dimethyl-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



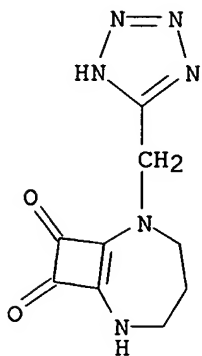
RN 144912-66-3 CAPLUS

CN Phosphonic acid, [3-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)propyl]- (9CI) (CA INDEX NAME)

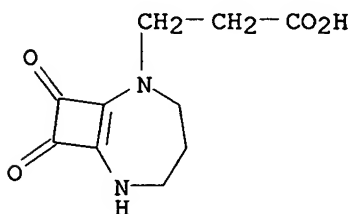


RN 144912-69-6 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione, 2-(1H-tetrazol-5-ylmethyl)- (9CI) (CA INDEX NAME)

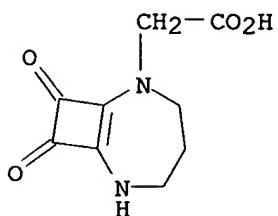


RN 144913-00-8 CAPLUS
 CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-propanoic acid, 8,9-dioxo-,
 monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 144913-01-9 CAPLUS
 CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetic acid, 8,9-dioxo-, monosodium
 salt (9CI) (CA INDEX NAME)



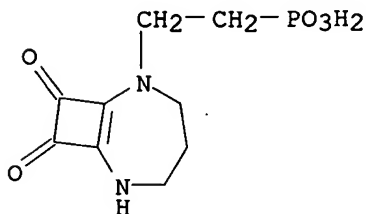
● Na

IT **144912-63-0P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)
 (design and synthesis of [(dioxodiazabicyclononenyl)ethyl]phosphonic

acid as a potent NMDA antagonist via use of cyclobutenedione as achiral amino acid bioisostere)

RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



IT 144912-83-4P 144912-87-8P 144912-92-5P

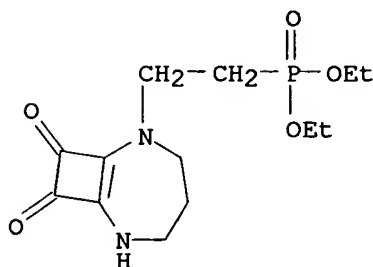
144912-99-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(design and synthesis of [(dioxodiazabicyclononenyl)ethyl]phosphonic acid as a potent NMDA antagonist via use of cyclobutenedione as achiral amino acid bioisostere)

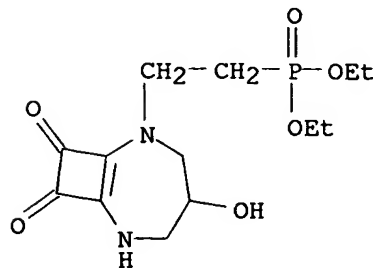
RN 144912-83-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 144912-87-8 CAPLUS

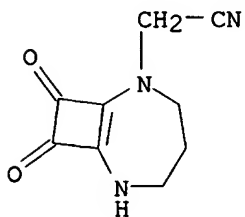
CN Phosphonic acid, [2-(4-hydroxy-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



10/820,216

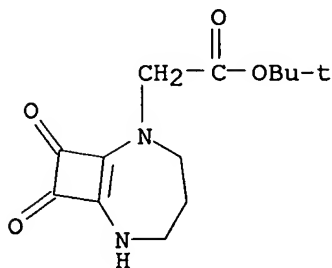
RN 144912-92-5 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetonitrile, 8,9-dioxo- (9CI) (CA INDEX NAME)



RN 144912-99-2 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetic acid, 8,9-dioxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

38

THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

✓
J11 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:5455 CAPLUS

DOCUMENT NUMBER: 126:74494

TITLE: Reaction of 3-morpholino-4-butoxy-3-cyclobutene-1,2-dione with amines

AUTHOR(S): Chen, Yizhao; Li, Jucai; Li, Wenzao; Yu, Lingzhuang; Hen, Linsen; Peng, Daquan

CORPORATE SOURCE: Dept. of Chemistry, Sichuan Univ., Chengdu, 610064, Peop. Rep. China

SOURCE: Sichuan Daxue Xuebao, Ziran Kexueban (1996), 33(3), 302-306

CODEN: SCTHAO; ISSN: 0490-6756

PUBLISHER: Sichuan Daxue Xuebao Bianjibu

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

AB When 3-morpholino-4-butoxy-3-cyclobutene-1,2-dione (I) reacted with amines, the reaction products were different depending on the nature of amines and the reaction conditions. In general, aminolysis of ester group took place, amino groups entered into the ortho position of 3-cyclobutene-1,2-dione. When 1,3-diaminopropane or m-aminophenol reacted with I, transamination of squaraines in intramol. and intermol. occurred in addition to aminolysis. The products formed in the reaction of o-aminophenol and o-phenylenediamine with I were not 1,2- rather 1,3-substituted squaramides.

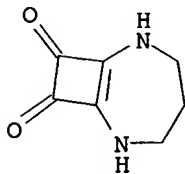
IT 66086-41-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(reaction of morpholino(butoxy)cyclobutenedione with amines)

RN 66086-41-7 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione (9CI) (CA INDEX NAME)



~~11~~ ANSWER 12 OF 17 CAPLUS COPYRIGHT, 2006 ACS on STN

ACCESSION NUMBER: 1993:39407 CAPLUS

DOCUMENT NUMBER: 118:39407

TITLE: Preparation of [[(2-amino-3,4-dioxo-1-cyclobuten-1-yl)amino]alkyl]carboxylic acid derivatives as N-methyl-D-aspartate (NMDA) antagonists

INVENTOR(S): Kinney, William Alvin; Garrison, Deanna Colette

PATENT ASSIGNEE(S): American Home Products Corp., USA

SOURCE: Eur. Pat. Appl., 33 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

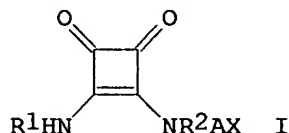
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 496561	A2	19920729	EP 1992-300472	19920120
EP 496561	A3	19921223		
EP 496561	B1	19950315		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, PT, SE				
US 5168103	A	19921201	US 1991-806861	19911217
IL 100679	A1	19961031	IL 1992-100679	19920116
AU 9210301	A1	19920730	AU 1992-10301	19920117
AU 639629	B2	19930729		
ZA 9200358	A	19930719	ZA 1992-358	19920117
SK 280268	B6	19991008	SK 1992-144	19920117
CZ 286407	B6	20000412	CZ 1992-144	19920117
CA 2059704	AA	19920723	CA 1992-2059704	19920120
CA 2059704	C	20020716		
JP 04321654	A2	19921111	JP 1992-7385	19920120
JP 3167770	B2	20010521		
AT 119873	E	19950415	AT 1992-300472	19920120
ES 2071428	T3	19950616	ES 1992-300472	19920120
RU 2039035	C1	19950709	RU 1992-5010645	19920120
FI 9200261	A	19920823	FI 1992-261	19920121
FI 105551	B1	20000915		
HU 61970	A2	19930329	HU 1992-192	19920121
HU 215838	B	20000628		
KR 206055	B1	19990701	KR 1992-780	19920121
US 5240946	A	19930831	US 1992-875925	19920429
PRIORITY APPLN. INFO.:			US 1991-644157	A 19910122
			US 1991-806861	A 19911217
			CS 1992-144	A 19920117

OTHER SOURCE(S): MARPAT 118:39407

GI



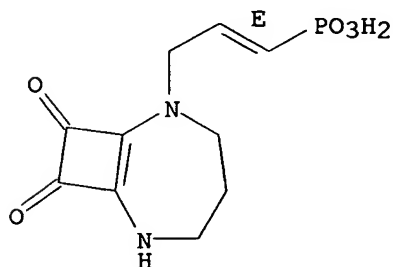
AB Title compds. [I; R1 = H, (phenyl)alkyl; R2 = R1, alkenyl; or R1R2 = CH2CH2, CH2CR6R7CH2, CH2CR8R9CR10R11CH2; R6, R8, R10 = H, alkyl, OH; R7, R9, R11 = H, alkyl; A = alkylene, alkenylene; X = CO2R3, P(O)(OR4)OR5, 3,5-dioxo-1,2,4-oxazolidin-2-yl, 5-tetrazolyl; R3, R4, R5 = H, alkyl], were prepared Thus, H2NCH2CH(OH)CH2NH2 was treated with O(CO2CMe3)2 in MeCN to give H2NCH2CH(OH)CH2NHCO2CMe3. The latter was condensed with BrCH2CH2P(O)(OEt)2 using Na2CO3 in EtOH to give (EtO)2P(O)CH2CH2NHCH2CH(OH)CH2NHCO2CMe3. This was condensed with 3,4-diethoxy-3-cyclobutene-1,2-dione in EtOH to give 3-[N-[2-(diethoxyphosphinyl)ethyl]-N-(2-ethoxy-3,4-dioxo-1-cyclobuten-1-yl)amino]-2-hydroxypropyl]carbamic acid 1,1-dimethylethyl ester. This was stirred with HCO2H and the residue was refluxed with EtN(CHMe2)2 in EtOH to give [2-(4-hydroxy-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid di-Et ester. This was refluxed with Me3SiBr in ClCH2CH2Cl to give [2-(4-hydroxy-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]phosphonic acid. The latter inhibited N-methyl-D-aspartate-induced lethality in mice with ED50 = 1.8 ng/kg.

IT 144912-54-9P 144912-55-0P 144912-63-0P
 144912-64-1P 144912-65-2P 144912-66-3P
 144912-67-4P 144912-68-5P 144912-69-6P
 144913-00-8P 144913-01-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as NMDA antagonist)

RN 144912-54-9 CAPLUS

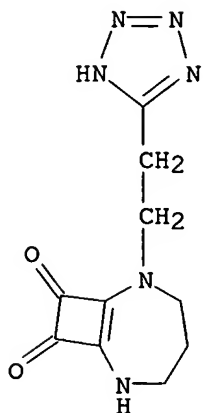
CN Phosphonic acid, [3-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)-1-propenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



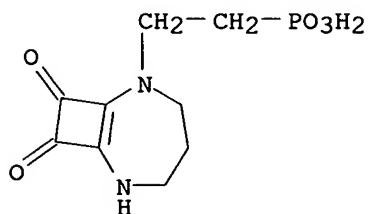
RN 144912-55-0 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione, 2-[2-(1H-tetrazol-5-yl)ethyl]- (9CI) (CA INDEX NAME)



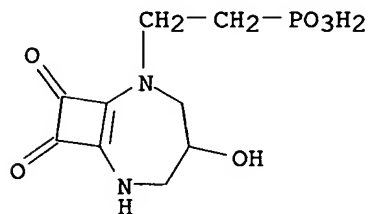
RN 144912-63-0 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



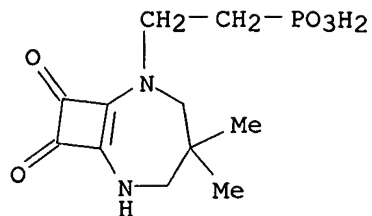
RN 144912-64-1 CAPLUS

CN Phosphonic acid, [2-(4-hydroxy-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



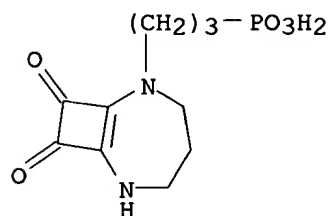
RN 144912-65-2 CAPLUS

CN Phosphonic acid, [2-(4,4-dimethyl-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]- (9CI) (CA INDEX NAME)



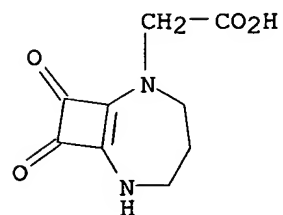
RN 144912-66-3 CAPLUS

CN Phosphonic acid, [3-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)propyl]- (9CI) (CA INDEX NAME)



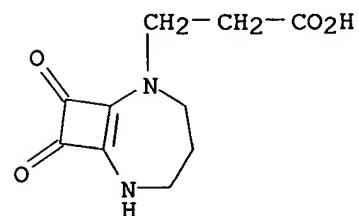
RN 144912-67-4 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetic acid, 8,9-dioxo- (9CI) (CA INDEX NAME)



RN 144912-68-5 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-propanoic acid, 8,9-dioxo- (9CI) (CA INDEX NAME)

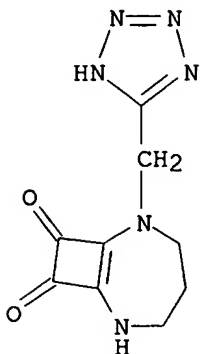


RN 144912-69-6 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione, 2-(1H-tetrazol-5-ylmethyl)-

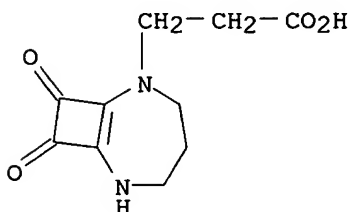
10/820,216

(9CI) (CA INDEX NAME)



RN 144913-00-8 CAPLUS

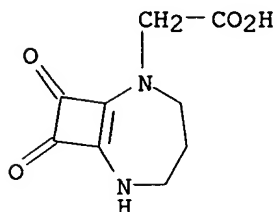
CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-propanoic acid, 8,9-dioxo-,
monosodium salt (9CI) (CA INDEX NAME)



● Na

RN 144913-01-9 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetic acid, 8,9-dioxo-, monosodium
salt (9CI) (CA INDEX NAME)



● Na

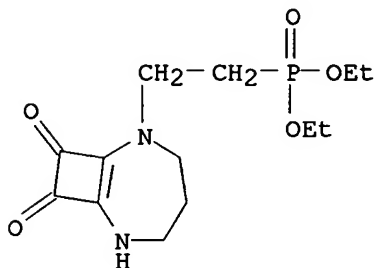
IT 144912-83-4P 144912-87-8P 144912-92-5P
144912-99-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for NMDA antagonists)

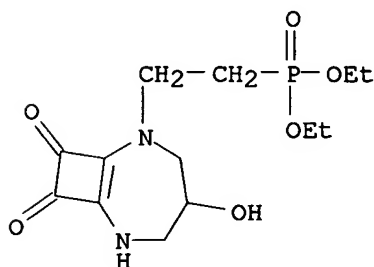
RN 144912-83-4 CAPLUS

CN Phosphonic acid, [2-(8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



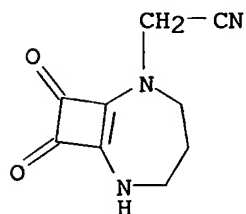
RN 144912-87-8 CAPLUS

CN Phosphonic acid, [2-(4-hydroxy-8,9-dioxo-2,6-diazabicyclo[5.2.0]non-1(7)-en-2-yl)ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



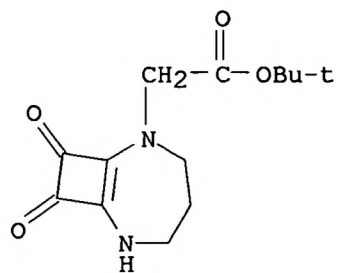
RN 144912-92-5 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetonitrile, 8,9-dioxo- (9CI) (CA INDEX NAME)



RN 144912-99-2 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-2-acetic acid, 8,9-dioxo-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



111 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1978:152588 CAPLUS

DOCUMENT NUMBER: 88:152588

TITLE: Ligand structure and complexation, XIV. Squaric acid and oxalic acid as building blocks of new crown ether amines and cryptands

AUTHOR(S): Voegtle, Fritz; Dix, Peter

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, Fed. Rep. Ger.

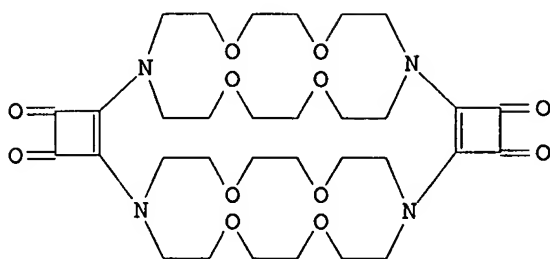
SOURCE: Justus Liebigs Annalen der Chemie (1977), (10), 1698-706

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



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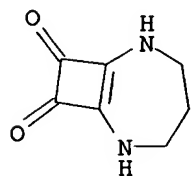
AB Aza crown ethers were prepared from squaric or oxalic acid and alkylenediamines or oxaalkylenediamines. I formed crystalline complexes with alkali metal ions.

IT **66086-41-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 66086-41-7 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-8,9-dione (9CI) (CA INDEX NAME)



111 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:579022 CAPLUS

DOCUMENT NUMBER: 83:179022

TITLE: Synthesis of heterocyclic compounds by condensation of 5-chloro-2-aminobenzhydramine with C1-C2 reagents

AUTHOR(S): Roth, H. J.; Mensel, H.

CORPORATE SOURCE: Pharm. Inst., Univ. Bonn, Bonn, Fed. Rep. Ger.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1975), 308(7), 557-63

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 83:179022

GI For diagram(s), see printed CA Issue.

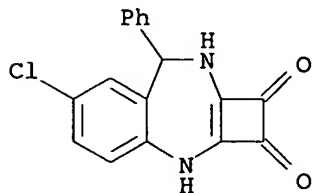
AB Condensation of 5,2-Cl(H₂N)C₆H₃CHPhNH₂ with RC(OEt)₃ (R = Me, Et), ClCOCOC₂H₄Cl, and 1,2-dimethoxycyclobutenedione gave quinazolines I, the macrocycle II, and the benzodiazepine III resp.

IT **57050-75-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 57050-75-6 CAPLUS

CN 1H-Benzo[e]cyclobuta[b][1,4]diazepine-1,2(3H)-dione, 6-chloro-8,9-dihydro-8-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1974:133399 CAPLUS

DOCUMENT NUMBER: 80:133399

TITLE: Polycarbonyl compounds. 7. Condensation of squaric acid 1,2-diamides with diethyl malonate

AUTHOR(S): Seitz, G.; Morck, H.

CORPORATE SOURCE: Chem. Inst., Tieraerztl. Hochsch. Hannover, Hanover, Fed. Rep. Ger.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1974), 307(2), 113-16

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

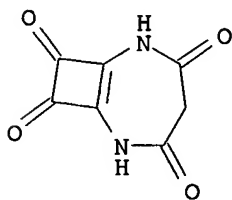
AB Condensation of the amides I (R = H or Me) with $\text{CH}_2(\text{CO}_2\text{Et})_2$ (in the case of R = H in the presence of EtONa) at reflux gave the diazabicyclononenes II.

IT 52094-04-9P 52094-06-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

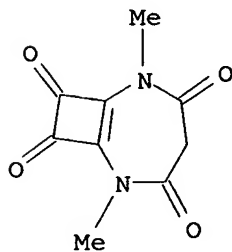
RN 52094-04-9 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-3,5,8,9-tetrone (9CI) (CA INDEX NAME)



RN 52094-06-1 CAPLUS

CN 2,6-Diazabicyclo[5.2.0]non-1(7)-ene-3,5,8,9-tetrone, 2,6-dimethyl- (9CI)
(CA INDEX NAME)



111 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:29271 CAPLUS

DOCUMENT NUMBER: 76:29271

TITLE: Spectroscopic and structural studies of some oxocarbon condensation products. V. Electronic structures of some cyclobuta[b]quinoxalines

AUTHOR(S): Griffiths, G. T.; Webb, G. A.

CORPORATE SOURCE: Dep. Chem. Phys., Univ. Surrey, Guildford/Surrey, UK

SOURCE: Journal of Molecular Structure (1971), 9(3), 333-42
CODEN: JMOSB4; ISSN: 0022-2860

DOCUMENT TYPE: Journal

LANGUAGE: English

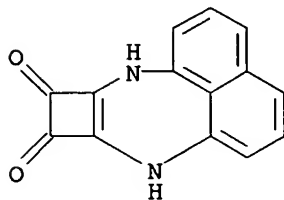
AB The electronic spectra of 12 cyclobuta[b]quinoxalines are reported and compared with electronic-transition energy and oscillator-strength values derived from Pariser-Parr-Pople MO calcns. The effects of nonplanarity on the electronic structures of these mols. are considered.

IT 33471-38-4

RL: PRP (Properties)

(electron configuration and electronic spectrum of, structure in relation to)

RN 33471-38-4 CAPLUS

CN Cyclobuta[b]naphtho[1,8-e,f][1,4]diazepine-8,9-dione, 7,10-dihydro- (9CI)
(CA INDEX NAME)

11 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1971:462688 CAPLUS

DOCUMENT NUMBER: 75:62688

TITLE: Spectroscopic and structural studies of some oxocarbon condensation products. IV. Spectroscopic and mass spectral investigation of some derivatives of squaric acid

AUTHOR(S): Griffiths, G. R.; Rowe, M. D.; Webb, G. A.

CORPORATE SOURCE: Dep. Chem. Phys., Univ. Surrey, Guildford/Surrey, UK

SOURCE: Journal of Molecular Structure (1971), 8(3), 363-71

CODEN: JMOSB4; ISSN: 0022-2860

DOCUMENT TYPE: Journal

LANGUAGE: English

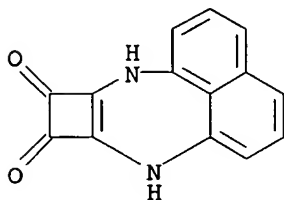
AB PMR, vibrational, and mass spectral data for nine mols. derived from squaric acid substantiate the cyclobuta[b] quinoxaline structure for six of the mols., whereas the others are simple derivs. of squaric acid.

IT **33471-38-4**

RL: PRP (Properties)

(spectrum of)

RN 33471-38-4 CAPLUS

CN Cyclobuta[b]naphtho[1,8-e,f][1,4]diazepine-8,9-dione, 7,10-dihydro- (9CI)
(CA INDEX NAME)

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